

[振動分配関数]

$$q_{\text{vib}}^{(1)} = \left[1 - \exp\left(-\frac{h\nu}{kT}\right) \right]^{-1} \quad \text{1 振動子 (7.4)}$$

$$q_{\text{vib-cl}}^{(1)} = \frac{kT}{h\nu} \quad \text{古典極限 1 振動子 (7.4-cl)}$$

$$q_{\text{vib}} = \prod_{i=1}^{n_v} \left[1 - \exp\left(-\frac{h\nu_i}{kT}\right) \right]^{-1} \quad n_v \text{ 振動子 (7.5)}$$

[回転分配関数]

$$q_{\text{rot}}^{2D} = \int_0^\infty \rho_{\text{rot}}^{2D} \exp\left(-\frac{\varepsilon_J}{kT}\right) d\varepsilon_J = \frac{kT}{\sigma B} \quad \text{2 次元回転子 (7.6)}$$

σ : 回転対称数
 = 2 (H₂, N₂, CO₂)
 = 1 (HCl, N₂O)

$$q_{\text{rot}}^{3D} = \frac{n_{\text{isom}} \pi^{1/2}}{\sigma} \left(\frac{kT}{A} \frac{kT}{B} \frac{kT}{C} \right)^{1/2} \quad \text{3 次元回転子 (7.7)}$$

σ : 回転対称数
 = 2 (H₂O, SO₂)
 = 3 (NH₃)
 :
 n_{isom} : (光学)異性体の数

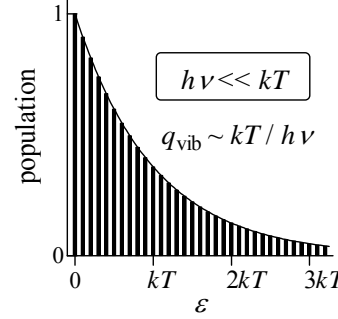
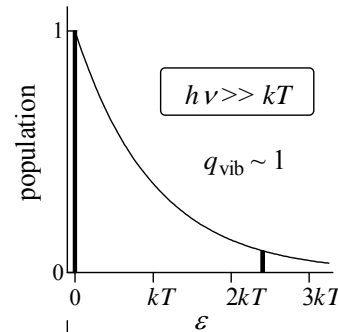
[並進分配関数]

$$q_{\text{trans}}^{1D} = \left(\frac{2\pi mkT}{h^2} \right)^{1/2} l \quad \text{1 次元並進 (7.8)}$$

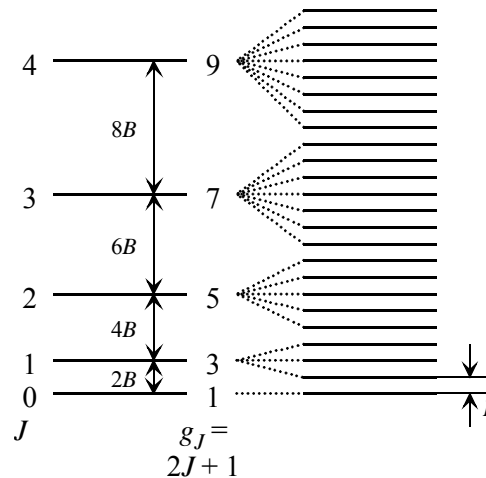
$$q_{\text{trans}}^{3D} = \left(\frac{2\pi mkT}{h^2} \right)^{3/2} l_x l_y l_z \quad \text{3 次元並進 (7.9)}$$

$$q_{\text{trans}}^\circ = \left(\frac{2\pi mkT}{h^2} \right)^{3/2} \quad \text{3 次元並進/単位体積あたり (7.10)}$$

$$q_{\text{trans}}^\circ = \left(\frac{2\pi \mu kT}{h^2} \right)^{3/2} \quad \text{3 次元相対並進/単位体積あたり (7.11)}$$



10.1 振動分配関数



10.2 二次元回転の状態密度 ~ 1/B

10.3

ボルツマン分布 - 統計力学的裏付

